

# High-order current correlation functions in Kondo systems.

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We examine the statistics of current fluctuations in a junction with a quantum dot described by Kondo Hamiltonian. With the help of modified Keldish technique we calculate the third current cumulant. As a function of ratio  $v = eV/T_K$  the 3rd cumulant was obtained for three different regimes: Fermi liquid regime ( $v < 1$ ), crossover interval ( $v \geq 1$ ) and RG limit ( $v \gg 1$ ). Unlike the case of noninteracting dot, 3rd cumulant shows strong non-linear voltage dependence. Only in the asymptotical limit  $v \rightarrow \infty$  the linear dependence on  $V$  is recovered.

PACS numbers: 72.10.Fk, 72.15.Qm, 73.63.Kv

*Motivation:* The direct electron transport is an important tool to study small junctions and quantum dots. The investigation of the current correlation functions helps to get additional information about physical properties of such systems. During last years the measurements only of the second cumulant of fluctuating current (shot noise) have resulted in a remarkable theoretical and experimental progress (see review article [1]). Interest in the third and higher moments has occurred, first, because its characteristics differ significantly from that of the second moment. In particular, as it was predicted by Levitov and Reznikov [2], in non-interacting systems the third moment is insensitive to the samples thermal noise, yet is more sensitive to the environment. Second, measurements of the higher moments may provide a new tool for studying conduction physics, complementary to the second moment. Experimentally it is quite nontrivial to extract cumulants higher then the second. Recently, however, the first experimental study of the third current cumulant in mesoscopic tunnel junctions was reported [3].

The theory of full counting statistic [4] is a theoretical framework which is used to analyze statistics of charge transfer in experiment and to calculate the higher order cumulants [5, 6]. However, when the interactions are included, which is the subject of the present paper, it is necessary to go beyond the theory of full counting statistics. Before starting such an analysis for Kondo type quantum dots we note that recently in a number of works third current cumulant in interacting mesoscopic systems was calculated [7, 8]. In these works the 3rd current cumulant was defined as a time ordered product of three current operators on standard Keldish 2-time contour. As a result this correlation function is equal to a sum of partially time ordered products on the usual one line time contour. Thus we can apply Feynman perturbation theory to evaluate this correlation function, however, we are unable for interacting systems to compute non-time ordered 3rd cumulant. It is important to resolve this discrepancy. Here with the help of a modified Keldish technique which uses a multiple time contour (see Fig.1)

[9] we directly provide such a derivation of non-time ordered 3rd cumulant for the Kondo problem.

*Hamiltonian. Third cumulant:* We start with the Kondo Hamiltonian for quantum dot in the junction  $H = H_L + H_R + H_J$  where

$$H_J = \sum_{\alpha\alpha'\sigma\sigma'} J_{\alpha\alpha'} c_{\alpha\sigma}^\dagger(0) \left( \frac{1}{4} \delta_{\sigma,\sigma'} + \vec{S} \vec{s}_{\sigma\sigma'} \right) c_{\alpha'\sigma'}(0) \quad (1)$$

The first two terms correspond to non-

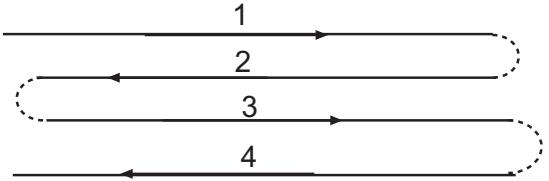


FIG. 1: The four-axis time contour

interacting electrons in the two leads  $H_{L(R)} = \sum_{k,\sigma} \xi_{L(R)k} c_{L(R)\sigma,k}^\dagger c_{L(R)\sigma,k}$ , where  $c_{\alpha\sigma,k}$ ,  $\xi_{\alpha k}$  are the electron field operator and the electron energy of a lead. Index  $\alpha = L, R$  indicates left (right) lead. We assume that the leads are dc-biased by applied voltage  $V$ . Here  $s$  is the one half spin matrix which acts on spin index of electron operators and  $S$  is the spin operator of the dot. The potential scattering is represented by the first term in the brackets. The bare coupling constants in (1) can be obtained by Schrieffer-Wolff transformation from the parent Anderson Hamiltonian

$$\begin{aligned} \hat{H} = & H_L + H_R + \sum_{k,\sigma,\alpha} (v_\alpha c_{\alpha\sigma,k}^\dagger d_\sigma + \text{H.c.}) \\ & + \sum_\sigma \epsilon d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow \end{aligned} \quad (2)$$

and are related to the parameters of this Hamiltonian [10] as  $J_{\alpha\alpha'} = \sqrt{\Gamma_\alpha \Gamma_{\alpha'}} / (\pi\nu|\tilde{\epsilon}|)$  and  $\tilde{\epsilon} \equiv (U - |\epsilon|)\epsilon/U$ . Here  $U$  is the repulsive Hubbard coupling,  $\epsilon$  denotes bare level energy of the dot and  $\nu$  is the density of states in a lead.

We also introduce the widths  $\Gamma_{L,R} = 2\pi\nu|v_{L,R}|^2$  which are expressed in terms of tunnelling matrix elements and density of electron states [11]. The current operator has a form

$$I = \frac{ie}{\hbar} [J_{LR} \sum_{\sigma\sigma'} c_{L\sigma}^\dagger(0) \left( \frac{1}{4} \delta_{\sigma,\sigma'} + \vec{S} \vec{s}_{\sigma\sigma'} \right) c_{R\sigma'}(0) - H.C.]$$

We define the 3rd momentum noise as a symmetric combination of non-time ordered correlation function of three currents. In a stationary situation this function can be written as

$$S_3(t_1 - t_2, t_2 - t_3) = \frac{1}{6} \sum_{P(\alpha\beta\gamma)} \langle I(t_\alpha) I(t_\beta) I(t_\gamma) \rangle \quad (3)$$

where  $P(\alpha\beta\gamma)$  is the permutation of 1,2,3. The Fourier-transformed value of (3)  $S_3(\omega_1, \omega_2)$  is a function of two energy variables. Below we consider the zero frequency limit  $S_3(\omega_1 = 0, \omega_2 = 0) \equiv S_3$  and introduce the third order cumulant  $S_3$ , that is, the irreducible part of correlation function (3). This cumulant yields the equation  $S_3 = S_3 - 3\bar{I}S_2 + 2\bar{I}^3$ . Here  $\bar{I}$  is the averaged current and  $S_2$  stands for the pair current correlation function (shot noise). In the Kondo regime this function was recently calculated [12].

*Perturbation theory. RG:* To apply perturbation theory to a product of non-time ordered Heisenberg operators like  $S_3$  we need to order these operators on some multiple time contour. For two operators (shot noise) the standard 2-time Keldysh contour is sufficient. However, to arrange more than two current operators additional time axis must be included. The 3rd order correlation function  $S_3$  is described by 4 lines contour (see Fig.1). [9]. The action consists of the integration over this four lines path. However, as it is common for Keldysh technique, we use only one infinite time path, though, with a four independent field operators, corresponding to the operators on each four branches (Fig.1) of complete time contour. Thus we have:

$$S = \frac{i}{\hbar} \int_{-\infty}^{\infty} dt \left[ \sum_{k\alpha\sigma} \hat{c}_{\alpha\sigma,k}^\dagger \hat{G}_{k\alpha}^{-1} \hat{c}_{\alpha\sigma,k} - \sum_{j=1}^4 \hat{\sigma}_z^j \hat{H}_j^j \right] \quad (4)$$

Here  $\hat{c}_{\alpha\sigma,k}^\dagger, \hat{c}_{\alpha\sigma,k}$  are the operators in  $4 \otimes 4$  Keldysh space,  $\hat{G}_{k\alpha}$  denotes  $4 \otimes 4$  Green's function of noninteracting leads;  $\sigma_z^j = 1$  if  $j=1,3$  and  $\sigma_z^j = -1$  if  $j=2,4$ . The interaction (1) now acquires Keldysh index  $j \rightarrow \hat{H}_j^j$ . We use the important equalities that relate the new Green functions on the contour in Fig.1. to the ordinary Keldysh Green functions defined on two lines contour. Keeping explicitly only Keldysh indices we can write them as:

$$\begin{aligned} G^{33} &= G^{11}, \quad G^{44} = G^{22} \\ G^{jj'} &= G^{12}, \quad j < j' \\ &= G^{21}, \quad j > j' \end{aligned} \quad (5)$$

On this four fold contour the correlation function is represented by time ordered product of three current operators

$$S_3(t_1 - t_2, t_2 - t_3) = \frac{1}{6} \sum_{P(ijk)} \langle T I^i(t_1) I^j(t_2) I^k(t_3) \rangle$$

Here superscripts  $i, j, k$  are corresponding Keldysh indices of the Heisenberg operators (electrons and spin  $\vec{S}$ ) related to the first three paths in Fig.1 (each index runs from 1 to 3). Summation over all permutations  $P$  of these indices is performed. Now we are ready to use non-equilibrium Keldysh technique and directly calculate  $S_3$ . In the lowest (fourth) non-vanishing order of perturbation theory in the coupling constant  $J_{\alpha,\alpha'}$  the zero-frequency irreducible correlation function  $S_3$  acquires a form:  $S_3 = S_3^{pot} + S_3^{pe} + S_3^{ex}$ , with  $S_3^{pot} = Y_{-1}/(2\hbar)$ ,  $S_3^{pe} = 9Y_{-1}/\hbar$  and  $S_3^{ex} = 3Y_7/(2\hbar)$  where

$$Y_n = \frac{\pi^3 e^3 g_{LR}^4}{4} \int d\omega (f_L - f_R) (f_L(1 - f_R) + f_R(1 - f_L) + n f_L f_R) \quad (6)$$

Here  $f_{L,R}$  are Fermi distribution functions for leads, and  $g_{\alpha\alpha'} = J_{\alpha\alpha'} \nu$  stand for dimensionless coupling constants. To mark the origin of different contributions we intentionally separate  $S_3$  into three parts: the first one  $S_3^{pot}$  represents potential scattering, the second part  $S_3^{pe}$  defines mixed exchange and potential interactions, while the last term  $S_3^{ex}$  stands for pure exchange scattering processes. For temperatures  $T \gg T_K$  ( $T_K \simeq D_0 \exp[-1/(g_{LL} + g_{RR})]$ ,  $D_0$  are the Kondo temperature and the effective bandwidth, correspondingly) logarithmic corrections which appear in perturbation theory can be disregarded. In this case the above formulae describe  $S_3$  as a function of source-drain voltage (see inset in Fig.2 where  $\underline{S} = S_3 e/T\sigma_B^2$  and  $\sigma_B = \pi e^2 g_{LR}^2/\hbar$  is the conductance in the Born approximation) for arbitrary values of the applied bias. It is interesting to note that unlike the case of noninteracting system a weak nonlinear voltage dependence of 3rd current cumulant at  $T \gg T_K$  persists in the lowest order of perturbation theory.

The logarithmic divergences appear in the next (fifth) order expansion in couplings  $g_{\alpha\alpha'}$ . We compute  $S_3$  to this order only for  $T = 0$ . In this case if voltages  $eV \gg T_K$  the perturbation theory still can be used. We keep only those fifth order terms that consist of the maximal logarithmic divergence. Only parts of  $S_3$  which include exchange tunnelling are affected by these logarithmic corrections, while the pure potential part of the three currents correlation function does not sufficiently change. Thus after long, though, direct calculations we arrive at

$$S_3^{pe} = \frac{9\pi^3}{4} \frac{e^4 V}{\hbar} g_{LR}^4 [1 + 2(g_{LL} + g_{RR}) \ln \frac{D_0}{eV}] \quad (7)$$

$$S_3^{ex} = \frac{3\pi^3}{8} \frac{e^4 V}{\hbar} g_{LR}^4 [1 + 4(g_{LL} + g_{RR}) \ln \frac{D_0}{eV}] \quad (8)$$

When the voltage is decreasing the log terms are starting to increase so that for  $eV \geq T_K$  the expansions (7,8) up to fifth order are not efficient. For this region 3rd momentum of the noise can be derived in the leading logarithmic approximation which consists of summation of the most diverging terms in each order in coupling constants  $g_{\alpha\alpha'}$ . From a set of equations (7,8) it becomes clear that the scaling behavior of  $S_3$  is similar to that of conductance [10]. This becomes particularly clear when we rewrite the expression for the 3rd noise in a following form:

$$S_3(T=0) = \pi V \left[ \frac{1}{8} \sigma_B^2 + 3\sigma_B \sigma_0(V) + \frac{2}{3} \sigma_0^2(V) \right] \quad (9)$$

where  $\sigma_0(V) = 3\pi e^2 [1 + 2(g_{LL} + g_{RR}) \ln(D_0/eV)]/(4\hbar)$  is the 'spin exchange' part of conductance, the part which includes logarithmic term. On the level of 'poor man's scaling technique in the zero temperature limit the renormalization proceeds till the band width  $D$  becomes equal to the applied bias  $eV$ . After that, the conductance can be calculated in the Born approximation with the renormalized exchange constant [10]:  $\sigma(V) = 3\pi e^2 \Gamma_L \Gamma_R / [2\sqrt{\hbar}(\Gamma_L + \Gamma_R) \ln(eV/T_K)]^2$ . The potential scattering contribution to conductance  $\sigma_B$  is not changed under RG transformations and renders a small correction to  $S_3$ . Thus, the final expression for the 3rd cumulant is given by equation (9) where we should replace  $\sigma_0(V)$  on  $\sigma(V)$ .

*Fermi liquid regime:* To study regime where  $T, eV < T_K$  we apply the mean field slave boson approximation (MFSB) [13]. The current operator for Anderson model acquires a form

$$I_s = \frac{ie}{2\hbar} \sum \int_{\sigma} [(v_L c_{L\sigma}^{\dagger}(0) - v_R c_{R\sigma}^{\dagger}(0)) d_{\sigma}(0) - H.C.] \quad (10)$$

In the slave-boson approach, the localized electron operator  $d_{\sigma}^{\dagger}$  is represented by  $\hat{f}_{\sigma}^{\dagger} \hat{b}$  with  $\hat{b}$  and  $\hat{f}_{\sigma}^{\dagger}$  being the standard boson and fermion operators. The total action on the time contour in Fig.1 has the similar form as (4). We should replace only  $H_J$  by interacting  $d$ -dependent part of the Anderson Hamiltonian (2). The two new terms in the action, equivalent to the first one in equation (4) come from slave bosons and auxiliary fermions Green's functions. Also the requirement of a single occupancy  $\hat{b}^{\dagger} \hat{b} + \sum_{\sigma} \hat{f}_{\sigma}^{\dagger} \hat{f}_{\sigma} = 1$  must be included into the action with a Lagrange multiplier. In the MFSB approximation the Bose operators  $\hat{b}^{\dagger}, \hat{b}$  are replaced by their expectation value  $b$ . We also add to the action the source term  $S_{\gamma} = \int dt \gamma^j(t) I_s^j$  ( $j$  is running from 1 to 4) and integrate out the fermion operators in the leads. Here  $I_s^j$  is the current operator for Anderson model taken on  $j$  branch of time contour in Fig.1. For a symmetric tunnelling ( $v_L = v_R = v, \Gamma_L = \Gamma_R = \Gamma$ ) the effective action can be written as  $S_{eff}(\gamma) = S_b + S_f$  where the first term is nonoperator bosonic part of the action, while the last

one explicitly depends on source fields  $\gamma^k(t)$  and is given by

$$\begin{aligned} S_f(\gamma) &= \sum_{\sigma} \int dt \int dt' \hat{f}_{\sigma}^{\dagger} [G_{d\sigma}^{-1}(\gamma)] \hat{f}_{\sigma} \\ G_{f\sigma}^{-1}(\gamma) &= G_{0f\sigma}^{-1} - T_k (Q^+ G_{L\sigma} Q^- + Q^- G_{R\sigma} Q^+) \quad (11) \\ G_{0f\sigma}^{-1}(\omega) &= (\omega - \tilde{\epsilon}) \hat{\sigma}_z, \quad Q_k^{\pm} = \hat{\sigma}_z^k \pm \frac{ie}{2\hbar} \gamma^k(t) \end{aligned}$$

Here  $G_{L,R}$  represents  $4 \otimes 4$  matrix of the electrons propagators in the leads,  $G_{0f\sigma}(\omega)$  is the Fourier transform of zero order slave fermions Green's function and  $\hat{\sigma}_z$  is diagonal  $4 \otimes 4$  matrix with elements  $\hat{\sigma}_z^j$  (4). We also define  $T_k = \Gamma b^2$  as an effective Kondo temperature. The  $G_{f\sigma}(\omega)$  includes the Lagrange multiplier which shifts the localized level position  $\epsilon$  to  $\tilde{\epsilon} = \epsilon + \lambda$ . Both free parameters  $T_k$  and renormalized level  $\tilde{\epsilon}$  are self-consistently determined by two equations that define the extremum of  $S_{eff}$  relative to  $b$  and  $\tilde{\epsilon}$  when  $U \rightarrow \infty$  [13].

We can trace out the slave fermions and get a closed form for generating functional:  $Z = \exp[-\frac{i}{2\hbar} \text{Tr} \ln G_f^{-1}(\gamma)]$ . The irreducible three currents correlation function or the 3rd cumulant is obtained by taking the third variation of the logarithm of this functional on source fields. Performing the straightforward calculations we find  $S_3 = S'_3 + S''_3$  where

$$\begin{aligned} S'_3 &= \frac{\pi e^3}{2} \int d\omega \rho^2(\omega) (f_L - f_R)^3 (3 - 4\pi T_k \rho(\omega)) \\ S''_3 &= \frac{\pi e^3}{2} \int d\omega \rho^2(\omega) (f_L - f_R) [1 - 3(f_L + f_R - 1)^2] \end{aligned}$$

Here the spectral density of interacting level  $\pi\rho(\omega) \equiv -\text{Im}G_d^r(\omega) = T_k/[(\omega - \tilde{\epsilon})^2 + T_k^2]$  is introduced. If  $T \rightarrow 0$  then 3rd cumulant becomes particularly simple. Expression for  $S_3$  is now reduced to

$$S_3 = \frac{2}{\pi} e^3 \int_0^{eV} d\omega T^2(\omega) (1 - T(\omega)) \quad (12)$$

where  $T(\omega) = \pi T_k \rho(\omega)$ . Thus, we obtain 3rd noise  $S_3$  as a function of two dimensionless parameters  $eV/T_k$  and  $\tilde{\epsilon}/T_k$ . A simple approximate expression for  $S_3$  follows when these parameters are small  $S_3 \approx 2e^6 V^3 / (3\pi T_k^2)$ . Such a voltage dependence is typical for a Fermi liquid.

*Discussion:* The crossover regime ( $T, eV \sim T_k$ ) actually is extended to a several threshold values  $T_K$ . This region can also be studied within the present theory by using non-crossing approximation in non-equilibrium (NCA)[14] together with  $1/N$  expansion for generating functional  $Z$ . A satisfied estimation of the 3rd noise in this case can be achieved by calculating equation (12) with a modified spectral density which is derived in NCA approximation:  $T_K \rho(\omega) \rightarrow \Gamma \rho_{NCA}(\omega)$ . We start numerical calculations by solving the mean field equations of MFSB theory. The MFSB method is limited to small voltages  $eV < T_K$  where it is known it gives the correct

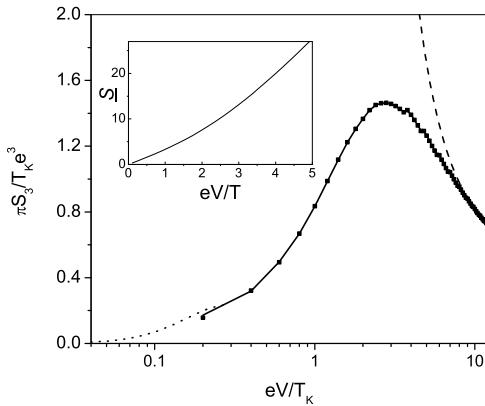


FIG. 2: The third cumulant  $S_3$  versus applied voltage  $eV/T_K$ . Dot curve represents MFSB calculations valid for small voltage  $eV < T_K$ . Solid line with black squares is obtained in NCA approximation. Dash line is the result of direct computation of Eq.(9) with  $\sigma_0 \rightarrow \sigma(V)$ . The curves which were calculated for two  $T_K$  differing by a factor of 10 practically coincide. This reflects the universality of 3rd cumulant in considered regime. (inset): Normalized 3rd cumulant  $\underline{S}$  as function of  $eV/T$  in the high temperature limit  $T \gg T_K$ .

qualitative behavior to this Fermi liquid regime. In addition, at  $eV \ll T_K$  the 3rd cumulant in MFSB approximation is matched with the perturbation theory derivation at the unitary limit of Kondo Hamiltonian. For conductance and noise calculations [12] the whole scheme with MFSB works rather well. At  $eV < T_K$  MFSB also gives adequate description of 3rd cumulant which is close to its exact value. The dot line in Fig.2 displayed the results of our MFSB calculations.

In the crossover region the NCA computations begin with a finite  $V$ . The main block which we need to calculate in NCA is  $\rho(\omega)$ . The 3rd current cumulant includes the frequency integration of different powers of  $\rho(\omega)$ . To estimate the accuracy of NCA we consider the known different physical values which are based on spectral density derivation. For example, for quantum dots, Cox [15] has shown that the calculated equilibrium susceptibility agree with the exact Bethe ansatz results to within the 0.5% convergence accuracy of the NCA. For the current calculations Wingreen and Meir (see [14]) use NCA equations in nonequilibrium and found at worse an overestimate of 15% on the linear response conductance. We expect the same (15%) accuracy for 3rd current cumulant. NCA result is given by solid curve with black squares in Fig.2. Strong nonlinearity with a peak at the intermediate voltage  $eV_m \sim 2.6T_K$  is determined by significant Kondo correlations. Indeed, in the absence of interacting  $S_3$  grows linearly with  $V$ . At  $eV \lesssim T_K$  we are in the strong Kondo regime where  $S_3$  grows considerably faster then simply linearly in  $V$ . The subsequent

decreasing of 3rd noise for  $V > V_m$  simply indicates on the weakening of the Kondo effect and manifests that Kondo correlations continues to determine the physics 3rd noise. Even when we go outside the crossover region and enter scaling limit  $D_0 \gg eV \gg T_K$  (dash line on Fig.2) where Kondo model is in a weak coupling regime with depressed Kondo effect,  $S_3$  shows a behavior which is far for being linear in  $V$ . Though, the Kondo effect is depressed, nevertheless, the logarithmic contributions to 3rd cumulant which in this region are related to Kondo correlations are considerably larger than those derived with the help of bare perturbation theory in the Born approximation. Linear or weak nonlinear voltage dependence which would be indicate the complete depression of Kondo correlations appears outside the domain of Fig.2 for bigger  $T$  (as inset in Fig2) or  $V$  ( $T, V \sim D_0$ ).

*Conclusions:* In conclusions, we have represented a general theory which allows to describe current fluctuations in quantum dot in the presence of interactions. In particular, we have considered a junction with quantum dot described by Kondo Hamiltonian. For this system we have calculated third cumulant of non-time ordered product of three current operators. Restricting ourselves to zero frequency we were able by our approach to cover three important regions: one is the in Fermi liquid limit, crossover regime, and weak coupling Kondo limit. Unlike the non-interaction system, in all cases  $S_3$  shows nonlinear voltage dependence. The linear dependence on  $V$  is restored only for large voltages  $V \rightarrow \infty$ . In this work we assumed that external impedance is equal to zero, the condition, which may be violated in the real experiment. This impedance leads to a modification of the third cumulant [16].

I would like to thank T. Martin for very helpful discussions and for drawing attention to the important work [9] and Yu. Nazarov for his suggestions related to the theory of full counting statistic. I also thankful to T. Aono, B. Horovitz, and Y. Meir for numerous discussions.

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